

1 What is claimed is:

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1 1. A computer-implemented method for generating a library design for a combinatorial
2 library of materials, comprising:

3 defining one or more sources and one or more destinations, each source being
4 electronic data representing a component to be used in preparing the combinatorial library
5 and each destination being electronic data representing an arrangement of cells;

6 receiving an input defining a first mapping, the first mapping being electronic data
7 defining a distribution pattern for assigning a component to cells in the arrangement, the
8 distribution pattern including a minimum and a maximum amount of the component to be
9 assigned to any cell of the arrangement and a gradient to be applied between the minimum
10 and maximum amounts of the component across the plurality of cells;

11 using the first mapping to calculate a composition of one or materials assigned to one
12 or more of the cells; and

13 generating a data file defining the library design, the data file comprising electronic
14 data representing the sources, the destinations and the mapping.

1 2. The method of claim 1, further comprising:

2 displaying a representation of the library design, the representation graphically
3 describing the composition of one or more materials assigned to one or more of the cells.

1 3. The method of claim 1, wherein the data file comprises electronic data representing
2 one or more sets of properties, each set of properties being associated with one of the
3 sources, the destinations or the mapping.

1 4. The method of claim 1, wherein defining the sources and destinations comprises
2 receiving an input from a graphical input device.

1 5. The method of claim 1, wherein the input defining a first mapping comprises a
2 selection from a set of available mapping types, the set of available mapping types
3 comprising a one to one mapping of a component from a source to a cell in the arrangement
4 and a one to many mapping of a component from a source to a plurality of cells in the
5 arrangement.

1 6. The method of claim 5, wherein the set of available mapping types further comprises
2 a many to many mapping of a plurality of components from a plurality of sources to a
3 plurality of cells in the arrangement.

1 7. The method of claim 6, wherein the set of available mapping types further comprises
2 a many to one mapping of a plurality of components from a plurality of sources to a cell in
3 the arrangement.

1 8. The method of claim 5, wherein the set of available mapping types further comprises
2 a set of one or more user-defined equations.

1 9. The method of claim 1, wherein the gradient is selected from the group consisting of
2 linear, logarithmic, exponential, polynomial and geometric progression.

1 10. The method of claim 3, wherein the set of properties associated with the mapping
2 comprises a source name, a source geometry, a destination name, a destination geometry, a
3 gradient type, and a set of gradient parameters defining the gradient.

1 11. The method of claim 1, further comprising:
2 receiving an input defining a second mapping, the second mapping being electronic
3 data defining a second distribution pattern for distributing a second component to cells in the
4 arrangement; and
5 using the first and second mappings to calculate a composition of one or more
6 materials assigned to one or more of the cells.

1 12. The method of claim 11, wherein the second distribution pattern for assigning a
2 second component includes electronic data identifying a fixed amount of the second
3 component to be assigned to one or more cells in the arrangement.

1 13. The method of claim 12, wherein the second distribution pattern for assigning a
2 second component includes electronic data identifying a minimum and a maximum amount
3 of the second component to be assigned to any of the cells of the arrangement and a second
4 gradient to be applied between the minimum and maximum amounts of the second
5 component across the cells.

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14. The method of claim 1, further comprising generating a modified library design by:
receiving an input redefining a source, a destination or a mapping;
recalculating the composition of one or more materials assigned to one or more of the
cells; and
generating a data file defining the modified library design.

15. The method of claim 1, further comprising:
receiving an input defining one or more parameters, each parameter being electronic
data corresponding to a process parameter and defining a parameter value for one or more
cells of the arrangement, the parameter value varying between a minimum and a maximum
amount; and
wherein the data file further comprises electronic data representing the one or more
parameters.

16. The method of claim 1, wherein the arrangement comprises two or more cells.

17. The method of claim 1, wherein the arrangement comprises ten or more cells.

18. The method of claim 1, wherein the arrangement comprises about ninety-six or more
cells.

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19. A computer-implemented method for generating a library design for a combinatorial
library of materials, comprising:

defining a set of one or more sources and one or more destinations, each source being
electronic data representing a component to be used in preparing the combinatorial library
and each destination being electronic data representing an arrangement of cells;

receiving an input defining a set of first mappings, the first mappings being electronic
data defining a set of equations for calculating an amount of one or more components to be
assigned to one or more cells in an arrangement;

using the set of equations to calculate a composition of a material assigned to one or
more of the cells; and

generating a data file defining the library design, the data file comprising electronic

1285 data representing the sources, the destinations and the mappings.

1 20. The method of claim 19, further comprising:
2 displaying a representation of the library design, the representation graphically
3 describing the composition of one or more materials assigned to one or more of the cells.

1 21. The method of claim 19, wherein the component to be assigned to a cell in the
2 arrangement is determined by the location of the cell within the arrangement.

1 22. The method of claim 21, wherein the composition of a material is determined using a
2 subset of the set of equations, the subset of equations being determined by the location of the
3 cell within the arrangement.

1 23. The method of claim 19, further comprising:
2 generating an error indicator signal if the number of equations in the set of equations
3 is not equal to the number of sources in the set of sources.

1 24. The method of claim 19, wherein at least one of the set of equations is selected from
2 the group consisting of:

3 a ratio equation defining an amount of a component to be assigned to a cell as a
4 function of an amount of another component to be assigned to the cell;

5 a volume equation defining an amount of a component to be assigned to a cell as a
6 function of a total volume of a plurality of components to be assigned to the cell; and

7 a mass equation defining an amount of a component to be assigned to a cell as a
8 function of a total mass of a plurality of components to be assigned to the cell.

1 25. The method of claim 19, wherein the set of equations comprises a gradient equation
2 defining an amount of a component to be assigned to each of a plurality of cells according to
3 a gradient.

1 26. The method of claim 19, wherein each of the set of equations is assigned to one or
2 more cells of the arrangement according to the location of the cells within the arrangement.

1 27. The method of claim 19, wherein using the set of equations to calculate a composition
2 of a material assigned to one or more of the cells comprises simultaneously solving a set of
3 interdependent equations.

1 28. The method of claim 27, wherein using the set of equations further comprises using a
2 matrix inversion technique to solve the set of equations.

1 29. The method of claim 19, further comprising:

2 receiving an input defining a second mapping, the second mapping being electronic
3 data defining a distribution pattern for distributing a component to cells in the arrangement,
4 the distribution pattern including a minimum and a maximum amount of the component to be
5 assigned to any cell of the cells of the arrangement and a gradient to be applied between the
6 minimum and maximum amounts of the component across the plurality of cells; and

7 using the first set of mappings and the second mapping to calculate a composition of
8 a material assigned to one or more of the cells.

1 Sub 30. A computer-implemented method for generating a library design for a combinatorial
2 B6 library of materials, comprising:

3 defining a set of one or more sources and one or more destinations, each source being
4 electronic data representing a component to be used in preparing the combinatorial library
5 and each destination being electronic data representing an arrangement of cells;

6 defining a plurality of mappings, the mappings in the aggregate defining a
7 composition for each of a plurality of materials assigned to a plurality of cells in the
8 arrangement;

9 receiving an input defining one or more parameters, each parameter being electronic
10 data corresponding to a process parameter and defining a parameter value for one or more
11 cells of the arrangement, the parameter value varying between a minimum and a maximum
12 amount; and

13 generating a data file defining the library design, the data file comprising electronic
14 data describing the source elements, the destination elements, the mappings and the
15 parameters.

1 31. The method of claim 30, wherein the parameter value is defined to vary over time.

2 32. The method of claim 30, wherein the parameter value is defined to vary across two or
3 more cells in the arrangement.

4 33. The method of claim 30, wherein the parameter value is defined to vary over time and

5 across two or more cells in the arrangement.

1 34. The method of claim 30, wherein the parameter value varies according to a gradient
2 selected from the group consisting of linear, logarithmic, exponential, polynomial and
3 geometric progression.

1 35. The method of claim 30, wherein the parameter value corresponds to a process
2 parameter selected from the group consisting of temperature, pressure, time, flow rate and
3 stirring speed.

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1 36. A computer-implemented method for preparing a combinatorial library of materials
2 on a substrate, the method comprising:
3 creating a library design by defining a set of design elements, the set of design
4 elements including one or more sources representing components to be used in preparing the
5 combinatorial library, one or more destinations, each destination comprising an arrangement
6 of one or more cells, and one or more elements selected from the group consisting of a
7 mapping defining a scheme for assigning one or more amounts of a component to one or
8 more cells of an arrangement and a parameter corresponding to a process parameter, the
9 parameter defining a parameter value for one or more cells of the arrangement, the parameter
10 value varying between a minimum and a maximum amount;
11 generating a data file comprising electronic data describing the sources, the
12 destinations, the mappings and the parameters; and
13 using the data file to cause an automated material handling apparatus to assemble the
14 combinatorial library on a substrate.

1 37. A computer program product on a computer-readable medium for generating a library
2 design for a combinatorial library of materials, the program comprising instructions operable
3 to cause a programmable processor to:
4 receive an input defining one or more sources and one or more destinations, each
5 source being electronic data representing a component to be used in preparing the
6 combinatorial library and each destination being electronic data representing an arrangement
7 of cells;
8 receive an input defining a first mapping, the first mapping being electronic data
9 defining a distribution pattern for assigning a component to cells in the arrangement, the

10 distribution pattern including a minimum and a maximum amount of the component to be
11 assigned to any cell of the arrangement and a gradient to be applied between the minimum
12 and maximum amounts of the component across the plurality of cells;

13 *B7* use the first mapping to calculate a composition of one or materials assigned to one or
14 more of the cells; and

15 generate a data file defining the library design, the data file comprising electronic data
16 representing the sources, the destinations and the mapping.

1 38. The computer program of claim 37, further comprising instructions operable to cause
2 a programmable processor to:

3 display a representation of the library design, the representation graphically
4 describing the composition of one or more materials assigned to one or more of the cells.

1 39. The computer program of claim 37, wherein the data file comprises electronic data
2 representing one or more sets of properties, each set of properties being associated with one
3 of the sources, the destinations or the mapping.

1 40. The computer program of claim 37, wherein the input defining the sources and
2 destinations comprises an input from a graphical input device.

1 41. The computer program of claim 37, wherein the input defining a first mapping
2 comprises a selection from a set of available mapping types, the set of available mapping
3 types comprising a one to one mapping of a component from a source to a cell in the
4 arrangement and a one to many mapping of a component from a source to a plurality of cells
5 in the arrangement.

1 42. The computer program of claim 41, wherein the set of available mapping types
2 further comprises a many to many mapping of a plurality of components from a plurality of
3 sources to a plurality of cells in the arrangement.

1 43. The computer program of claim 42, wherein the set of available mapping types
2 further comprises a many to one mapping of a plurality of components from a plurality of
3 sources to a cell in the arrangement.

1 44. The computer program of claim 40, wherein the set of available mapping types

2 further comprises a set of one or more user-defined equations.

1 45. The computer program of claim 37, wherein the gradient is selected from the group
2 consisting of linear, logarithmic, exponential, polynomial and geometric progression.

1 46. The computer program of claim 39, wherein the set of properties associated with the
2 mapping comprises a source name, a source geometry, a destination name, a destination
3 geometry, a gradient type, and a set of gradient parameters defining the gradient.

1 47. The computer program of claim 37, further comprising instructions operable to cause
2 a programmable processor to:

3 receive an input defining a second mapping, the second mapping being electronic
4 data defining a second distribution pattern for distributing a second component to cells in the
5 arrangement; and

6 use the first and second mappings to calculate a composition of one or more materials
7 assigned to one or more of the cells.

1 48. The computer program of claim 47, wherein the second distribution pattern for
2 assigning a second component includes electronic data identifying a fixed amount of the
3 second component to be assigned to one or more cells in the arrangement.

1 49. The computer program of claim 48, wherein the second distribution pattern for
2 assigning a second component includes electronic data identifying a minimum and a
3 maximum amount of the second component to be assigned to any of the cells of the
4 arrangement and a second gradient to be applied between the minimum and maximum
5 amounts of the second component across the cells.

1 50. The computer program of claim 37, further comprising instructions operable to cause
2 a programmable processor to generate a modified library design by receiving an input
3 redefining a source, a destination or a mapping; recalculating the composition of one or more
4 materials assigned to one or more of the cells; and generating a data file defining the
5 modified library design.

1 51. The computer program of claim 37, further comprising instructions operable to cause
2 a programmable processor to:

3 receive an input defining one or more parameters, each parameter being electronic
4 data corresponding to a process parameter and defining a parameter value for one or more
5 cells of the arrangement, the parameter value varying between a minimum and a maximum
6 amount; and

7 wherein the data file further comprises electronic data representing the one or more
8 parameters.

1 *B1* 52. The computer program of claim 37, wherein the arrangement comprises two or more
2 cells.

1 53. The computer program of claim 37, wherein the arrangement comprises ten or more
2 cells.

1 54. The computer program of claim 37, wherein the arrangement comprises about ninety-
2 six or more cells.

1 55. A computer program product on a computer-readable medium for generating a library
2 design for a combinatorial library of materials, the program comprising instructions operable
3 to cause a programmable processor to:

4 receive an input defining a set of one or more sources and one or more destinations,
5 each source being electronic data representing a component to be used in preparing the
6 combinatorial library and each destination being electronic data representing an arrangement
7 of cells;

8 receive an input defining a set of first mappings, the first mappings being electronic
9 data defining a set of equations for calculating an amount of one or more components to be
10 assigned to one or more cells in an arrangement;

11 use the set of equations to calculate a composition of a material assigned to one or
12 more of the cells; and

13 generate a data file defining the library design, the data file comprising electronic data
14 representing the sources, the destinations and the mappings.

1 56. The computer program of claim 55, further comprising instructions operable to:

2 display a representation of the library design, the representation graphically

3 describing the composition of one or more materials assigned to one or more of the cells.

1 57. The computer program of claim 55, wherein the component to be assigned to a cell in
2 the arrangement is determined by the location of the cell within the arrangement.

1 58. The computer program of claim 57, wherein the composition of a material is
2 determined using a subset of the set of equations, the subset of equations being determined
3 by the location of the cell within the arrangement.

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1 59. The computer program of claim 55, further comprising instructions operable to:
2 generate an error indicator signal if the number of equations in the set of equations is
3 not equal to the number of sources in the set of sources.

1 60. The computer program of claim 55, wherein at least one of the set of equations is
2 selected from the group consisting of:

3 a ratio equation defining an amount of a component to be assigned to a cell as a
4 function of an amount of another component to be assigned to the cell;

5 a volume equation defining an amount of a component to be assigned to a cell as a
6 function of a total volume of a plurality of components to be assigned to the cell; and

7 a mass equation defining an amount of a component to be assigned to a cell as a
8 function of a total mass of a plurality of components to be assigned to the cell.

1 61. The computer program of claim 55, wherein the set of equations comprises a gradient
2 equation defining an amount of a component to be assigned to each of a plurality of cells
3 according to a gradient.

1 62. The computer program of claim 55, wherein each of the set of equations is assigned
2 to one or more cells of the arrangement according to the location of the cells within the
3 arrangement.

1 63. The computer program of claim 55, wherein the instructions operable to cause a
2 programmable processor to use the set of equations to calculate a composition of a material
3 assigned to one or more of the cells comprise instructions simultaneously to solve a set of
4 interdependent equations.

1 64. The computer program of claim 63, wherein the instructions simultaneously to solve
2 the set of interdependent equations further comprise instructions to use a matrix inversion

3 technique to solve the set of equations.

1 65. The computer program of claim 55, further comprising instructions operable to:

2 receive an input defining a second mapping, the second mapping being electronic

3 data defining a distribution pattern for distributing a component to cells in the arrangement,

4 the distribution pattern including a minimum and a maximum amount of the component to be

5 assigned to any cell of the cells of the arrangement and a gradient to be applied between the

6 minimum and maximum amounts of the component across the plurality of cells; and

7 use the first set of mappings and the second mapping to calculate a composition of a

8 material assigned to one or more of the cells.

1 66. A computer program product on a computer-readable medium for generating a library
2 design for a combinatorial library of materials, the program comprising instructions operable
3 to cause a programmable processor to:

4 receive an input defining a set of one or more sources and one or more destinations,

5 each source being electronic data representing a component to be used in preparing the

6 combinatorial library and each destination being electronic data representing an arrangement
7 of cells;

8 receive an input defining a plurality of mappings, the mappings in the aggregate
9 defining a composition for each of a plurality of materials assigned to a plurality of cells in
10 the arrangement;

11 receive an input defining one or more parameters, each parameter being electronic
12 data corresponding to a process parameter and defining a parameter value for one or more
13 cells of the arrangement, the parameter value varying between a minimum and a maximum
14 amount; and

15 generate a data file defining the library design, the data file comprising electronic data
16 describing the source elements, the destination elements, the mappings and the parameters.

1 67. The computer program of claim 66, wherein the parameter value is defined to vary
2 over time.

1 68. The computer program of claim 66, wherein the parameter value is defined to vary
2 across two or more cells in the arrangement.

1 69. The computer program of claim 66, wherein the parameter value is defined to vary
2 B7 over time and across two or more cells in the arrangement.

1 70. The computer program of claim 66, wherein the parameter value varies according to a
2 gradient selected from the group consisting of linear, logarithmic, exponential, polynomial
3 and geometric progression.

1 71. The computer program of claim 66, wherein the parameter value corresponds to a
2 process parameter selected from the group consisting of temperature, pressure, time, flow
3 rate and stirring speed.

1 72. A computer program product on a computer-readable medium for generating a library
2 design for a combinatorial library of materials, the program comprising instructions operable
3 to cause a programmable processor to:

4 create a library design by defining a set of design elements, the set of design elements
5 including one or more sources representing components to be used in preparing the
6 combinatorial library, one or more destinations, each destination comprising an arrangement
7 of one or more cells, and one or more elements selected from the group consisting of a
8 mapping defining a scheme for assigning one or more amounts of a component to one or
9 more cells of an arrangement and a parameter corresponding to a process parameter, the
10 parameter defining a parameter value for one or more cells of the arrangement, the parameter
11 value varying between a minimum and a maximum amount;

12 generate a data file comprising electronic data describing the sources, the
13 destinations, the mappings and the parameters; and

14 use the data file to cause an automated material handling apparatus to assemble the
15 combinatorial library on a substrate.